**MS Project in Computation and Machine Learning:**  
**AI-Guided Discovery of Smart 2D Materials**

Paulette Clancy Research Group. [https://clancygroup.wse.jhu.edu](https://clancygroup.wse.jhu.edu/)  
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This project is well suited for a master’s student with an interest in computational materials science, machine learning, and next-generation electronics. The goal is to explore how different “building blocks”—including transition-metal dopants, heteroatoms, and even organic intercalants—can be inserted into layered van der Waals (vdW) materials to flexibly reconfigure their structure and properties, much like assembling a customizable Lego set. By controlling defect motion and intercalation, we aim to unlock new routes for tuning electronic, thermal, and mechanical behaviors in 2D heterostructures.

The student will use Density Functional Theory (DFT) with the open-source Quantum ESPRESSO codebase, together with emerging machine learning approaches, to study migration pathways, stability, and property modulation in doped or intercalated 2D materials. While our current focus is on Cr-intercalated Sb2Te3, this framework naturally extends to a wide design space of atoms, molecules, and polymers as programmable “atomic glue” for vdW systems. An exciting future direction is to train machine learning models to predict migration barriers and property changes from simple physical descriptors such as vdW gap size, enabling rapid screening of reconfigurable 2D materials for applications in adaptive electronics, spintronics, and thermoelectrics.

This project offers students hands-on experience with both quantum simulations and AI-driven discovery, while contributing to a new paradigm in materials engineering—moving from designing static compounds to designing dynamic, reconfigurable systems. It provides excellent preparation for careers in materials informatics, energy applications, and advanced graduate research.

If interested, please send your CV to Paulette Clancy [PCLANCY3@jhu.edu](mailto:PCLANCY3@jhu.edu)